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Spectrochimica Acta Part B 50 (1995) 1637–1654

SPECTROCHIMICA ACTA
PART B

Three-dimensional modelling of the analyte dynamics in electrothermal atomizers for analytical spectrometry: influence of physical factors[1]

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Received 10 March 1995; accepted 24 May 1995

Abstract

A computer model has been developed that allows the calculation of the three-dimensional distributions of free atoms and condensed particles inside tube-type electrothermal atomizers. This model is a numerical solution of the three-dimensional diffusion equation written with the appropriate boundary conditions. The proposed model takes the following geometrical and physical factors into account: real tube geometry of an atomizer provided with a dosing hole, analyte vaporization, the size of the region occupied by the sample prior to atomization, three-dimensional analyte diffusion in a non-isothermal furnace environment, and its gas phase (homogeneous) condensation at the cooler parts of the atomizer. The physical processes that take place in electrothermal atomizers are common to all analytes and are the background against which chemical processes take place. Silver was used as the test element for modelling because Ag is a relatively inert element in electrothermal atomization, for which physical processes can be expected to dominate over chemical processes. Imaged representations of the calculated three-dimensional distributions of free Ag atoms and condensed Ag micro-droplets within Perkin-Elmer HGA-type atomizers are given. The imaged representations show that, even for a relatively inert element such as silver, the distribution of atoms in electrothermal atomizers is quite non-homogeneous.

Keywords: Computer modelling; Condensation; Electrothermal atomization; Spatial distribution of analyte

1. Introduction

For a long time after the introduction of the graphite furnace into analytical practice by L'vov [1] there was no spatial resolution to the measurements that were made. Only single atomic absorbance profiles were available and there was no information about the analyte's

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[1] This paper has been published in the special issue of the East European Furnace Symposium, 4–7 September 1994, Warsaw, Poland.

SSDI 0584-8547(95)01365-2